MCNPX Advances for Accelerator Applications

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Abstract - *MCNPX is the Monte Carlo N-Particle eXtended version of MCNP. MCNPX transports 34 different particle types up to the terravolt energy range and was originally developed specifically for accelerator applications. In the past 2 years, many significant advances have been made that are of particular interest to the accelerator community. The upgrade to MCNP4C includes delayed neutrons, unresolved resonance range probability tables for neutron cross sections, extensions to ENDF/B-VI formats, and an electron physics upgrade. Also available from MCNP4C are superimposed-mesh weight windows, macrobody geometries, and interactive geometry plotting. MCNPX is now fully PC compatible with both Windows and Linux and supports distributed memory multiprocessing for the entire range of all particles. There are also many entirely new capabilities. MCNPX has been modernized to F90. Color geometry plots allow 64 colors and coloring by most parameters. Photonuclear data and proton cross sections now may be plotted. Many user conveniences have been added, such as default dose functions, logarithmic interpolation of tally bins, and easier source specification. Physics enhancements include positron sources, a spontaneous fission model, fission multiplicity, ^{3}He coincidence modeling, and light-ion recoil. The MCNPX CEM physics model has been upgraded from CEM95 to CEM2k and a photonuclear physics model has been added. MCNPX can now mix and match physics models and data tables. It is now possible to specify some nuclides with models and other nuclides with data tables. It is also possible to use data tables up to their maximum energy value and then use models above that energy, even when the maximum table energy differs from nuclide to nuclide.*

I. INTRODUCTION

MCNPX [1,2] is the Monte Carlo N-Particle eXtended version of MCNP[3]. MCNPX transports 34 different particle types up to the TeV energy range and was originally developed for the Accelerator Production of Tritium program. Recent improvements have also been made for the Advanced Fuel Cycle program, NASA, and Homeland Defense.

In the past 2 years, several significant advances have been made that are of particular interest to the accelerator community. First we describe the infrastructure advances, including Fortran 90 (F90) modernization, PC support, and distributed memory multiprocessing. Then we describe the two major new enhancements of interest to the accelerator community, Cascade-Exciton Model (CEM) 2k physics and the new mix-and-match capability. Finally we describe projects in progress and future plans.

II. INFRASTRUCTURE ADVANCES

Several significant capabilities have been added to MCNPX in the past 2 years. MCNPX 2.4.0 was released to the Radiation Safety

Information and Computational Center (RSICC) in Oak Ridge, Tennessee, in August 2002. MCNPX 2.4.0 is based on MCNP4C3 [4,5], the latest RSICC MCNP version at the time of this writing. Physics capabilities inherited from MCNP4C3 include delayed neutrons, unresolved resonance range probability tables for neutron cross sections, extensions to ENDF/B-VI data representations, and an upgrade of the electron physics model to the Integrated Tiger Series [6] (ITS) Version 3.0.

Non-physics enhancements inherited from the MCNP4C upgrade include superimposed-mesh weight windows, macrobody geometries, and interactive geometry plotting. The superimposed-mesh weight windows technique enables variance reduction on a rectangular or cylindrical mesh superimposed over the problem geometry. The weight window importance functions can be generated interactively by successive MCNPX calculations. No longer is it necessary to subdivide geometries into many problem cells to do variance reduction.

Macrobody geometries enable specification of problem geometries with combinatorial-type bodies. These bodies are fully compatible with the MCNPX surface-sense geometry specification and greatly simplify problem setup. The bodies follow the body description conventions of the ITS [6] code.

The interactive geometry plotting, also inherited from MCNP4C, enables point-and-click plotting of problem geometries and superimposed meshes. The old command-prompt geometry plotting mode is still fully functional but no longer necessary.

MCNPX is now fully PC compatible with both Windows and Linux. In addition, standard UNIX platforms are supported.

MCNPX supports distributed memory multiprocessing for the entire range of all particles. Parallel Virtual Machine (PVM) and Message Passing Interface (MPI) standard software can be used to run the entire MCNPX code in parallel. Fault tolerance and load balancing are available, and multiprocessing can be done across a network of heterogeneous platforms. Threading may be used for problems run in the table data region only.

Several new MCNPX features provide capabilities beyond what is available in MCNP4C3. MCNPX has been modernized to Fortran-90, enhancing its compatibility with modern compilers and enabling better dynamic allocation of storage. The F90 conversion provides improvements in code modularity, standardization of functions such as timing across platforms, and compiler reliability. As much of MCNP4C3 has been preserved as possible to both maintain code integrity and maintain compatibility with the many existing "patches" in the user community. Most user patches still apply without modification.

The MCNPX plotting capabilities have been further enhanced. Color geometry plots now allow 64 colors and coloring by most parameters instead of just material. Photonuclear data and proton cross sections now may be plotted. A pause command is available with tally and cross-section plots.

Many user conveniences have been added, such as default dose functions, logarithmic interpolation of tally bins, and easier source specification. The latest code release also includes a capability to superimpose the 'i,j,k' lattice indices directly on the geometry plot.

Physics enhancements include positron sources, a spontaneous fission model, fission multiplicity, ^{3}He coincidence modeling, positron sources, and light-ion recoil.

III. CEM2K PHYSICS

The MCNPX CEM physics model has been upgraded from CEM95 to CEM2k [7]. The model assumes that reactions occur in three stages. The first stage is the Intra Nuclear Cascade (INC), in which primary particles can be re-scattered and produce secondary particles several times before absorption by or escape from the nucleus. The excited residual nucleus remaining after the cascade determines the particle-hole configuration that is the starting point for the pre-equilibrium stage of the reaction. The subsequent relaxation of the nuclear excitation is treated in terms of an improved Modified Exciton Model of pre-equilibrium decay followed by the equilibrium evaporative final stage of the reaction, which is competing with the fission and Fermi-breakup channels.

CEM2k incorporates new approximations for the elementary cross sections used in the cascade, using more precise values for nuclear masses and pairing energies, corrected systematics for the level-density parameters, and several other refinements. Improved algorithms decrease the computing time by up to a factor of six for heavy targets. Other improvements were motivated by new measured data on isotope production from GSI experiments. CEM2k has a longer cascade state, less preequilibrium emission, and evaporation from more highly excited compound nuclei as compared with earlier versions. CEM2k also has better models of neutron, radionuclide, and gas production in accelerator-transmutation-of-waste spallation targets.

A photonuclear physics package has been added to CEM2k for photon energies from 8 MeV to about 2 GeV, and includes the Giant Dipole and Quasi-Deuteron resonances. These photonuclear physics models compliment existing photonuclear data evaluations in that they may be used for nuclides where no tabular data exist. Also, they may be used for tabular-data nuclides above the 150-MeV upper-energy boundary of the tables.

IV. MIX-AND-MATCH CAPABILITY

MCNPX can now mix and match physics models and data tables. It is now possible to specify some nuclides with models and other nuclides with data tables (isotope 'mixing'). It is also possible to use data tables up to their maximum energy value and then use models above that energy, even when the maximum table energy differs from nuclide to nuclide ('energy matching') [8].

As an example, consider protons interacting with a Bismuth Germinate particle detector (BGO). Because the present LA-150 nuclear data libraries [9] do not include Germanium, it was previously possible to use only physics models for all nuclides in the entire problem. With the mix-and-match capability, Bismuth and Oxygen can be modeled with the more accurate nuclear data tables, whereas Germanium utilizes a physics model.

As another example, consider a neutron problem with Deuterium and Tritium. The available Deuterium library goes up to 150 MeV, but the Tritium library goes up to only 20 MeV. Previously, either neutron physics models above 20 MeV (neglecting the Deuterium table data up to 150 MeV) or nuclear data tables below 150 MeV (using the 20-MeV Tritium data throughout the entire 20-MeV to 150-MeV range) had to be used. With the mix-and-match capability, Deuterium uses tables up to 150 MeV and uses physics models above 150 MeV; Tritium uses data tables up to 20 MeV and uses physics models above 20 MeV.

Figure 1 shows an example of the energy matching capability. 100 MeV neutrons are incident on a 8.433 cm long, 3.932 cm radius BGO crystal. The crystal contains 21% Bi, 16% Ge and 63% O. No Ge libraries are currently available. The solid line represents flux in the crystal with the full mix and match capability, which uses all libraries up to their energy limits, and physics models above those limits and for Ge. The dashed line calculation uses the old method of substituting Arsenic for the missing Ge library, using the libraries up to 20 MeV, and using physics models above. The dotted line uses Bi and O libraries up to their limits of 150 MeV; the As library is used up to its limit of 20 MeV, and then the 20 MeV data is used from 20-150 MeV; above 150 MeV physics models are used for all three nuclides. This last option is least desirable, but was often used in past code versions to take advantage of the 150 MeV libraries, even though many data libraries only go to 20 MeV.

The mix-and-match capability is particularly useful for photonuclear calculations because few photonuclear data tables are currently available. Now libraries are used when available and models are used otherwise. Note that photonuclear physics is modeled with the new CEM2k model, regardless of whether CEM is used for other particles.

It is also possible now to substitute different nuclides for different particle types. For example, natural Carbon and Calcium can be used for neutrons and ^{12}C and ^{40}Ca can be used for protons and photonuclear reactions.

V. PRESENT AND FUTURE PROJECTS

Present MCNPX development projects include the following:

- implementation of theINCL4 (Intra Nuclear Cascade Liege) physics also known as the Cugnon INC and Schmidt evaporation physics models;
- special features for space applications, particularly anticoincidence detector models and gamma-line sources;
- weight windows and other variance reduction methods fully extended to physics models. Forced collisions, DXTRAN, next-event estimators and other techniques would be limited to neutral particles;
- secondary particle angle biasing for isotropic distributions;
- multiple source particle types;
- pulse height tallies with variance reduction; and
- neutral particle perturbation techniques extended to physics model region;

The following projects are planned:

- coupling MCNPX with burnup calculations and isotopic depletion;
- interactive tally and cross-section plotting;
- integration of HTAPE tallies directly into MCNPX;
- improved high-energy physics with the LAQGSM model;
- Addition of CINDER modules for transmuation applications;
- heavy ion tracking and interactions; and
- computer-aided design (CAD) interface.

We believe that the implementation of these and other new features will keep MCNPX at the forefront of accelerator application computer modeling capabilities.

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Fig. 1. Neutron flux in BGO